Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 11:03 AM EDT

PDB ID	:	3TPU
Title	:	42F3 p5E8/H2-Ld complex
Authors	:	Adams, J.J.; Kranz, D.M.; Garcia, K.C.
Deposited on	:	2011-09-08
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

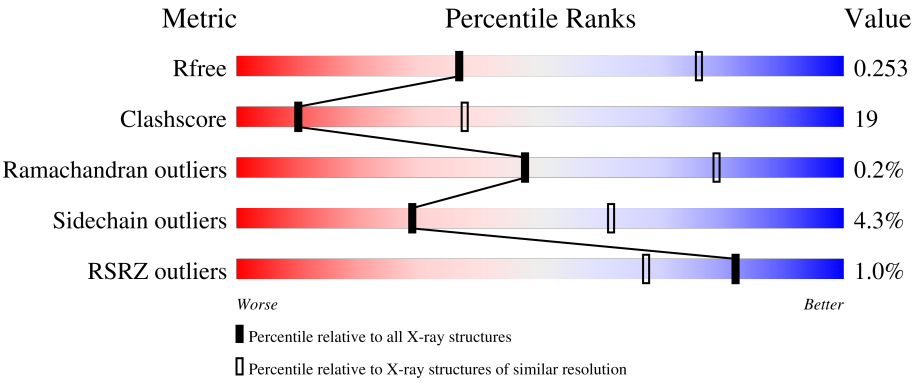
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	211	58% 35%
1	C	211	% 60% 35%
1	G	211	3% 63% 31%
1	M	211	2% 57% 37%
2	B	243	73% 25%

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Mol	Chain	Length	Quality of chain
2	D	243	69% 28%
2	H	243	2% 68% 29%
2	N	243	% 68% 28%
3	E	180	63% 33%
3	I	180	% 56% 37%
3	K	180	67% 27%
3	Q	180	2% 62% 35%
4	F	9	44% 56%
4	J	9	44% 56%
4	L	9	56% 44%
4	R	9	67% 22% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	E	180	-	-	X	-
5	SO4	N	243	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20148 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 42F3 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1595	1007	264	316	8			
1	C	204	Total	C	N	O	S	0	0	0
			1584	1000	262	314	8			
1	G	202	Total	C	N	O	S	0	0	0
			1573	994	261	310	8			
1	M	204	Total	C	N	O	S	0	0	0
			1587	1001	263	315	8			

- Molecule 2 is a protein called 42F3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	0	0	0
			1900	1197	330	367	6			
2	D	240	Total	C	N	O	S	0	0	0
			1900	1197	330	367	6			
2	H	240	Total	C	N	O	S	0	0	0
			1900	1197	330	367	6			
2	N	240	Total	C	N	O	S	0	0	0
			1900	1197	330	367	6			

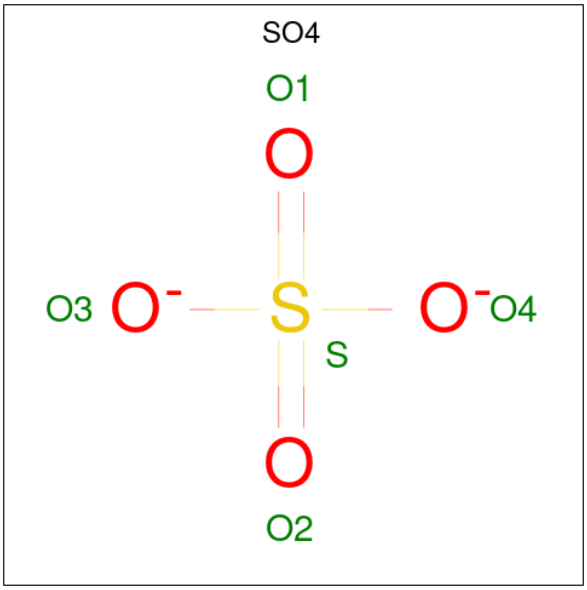
- Molecule 3 is a protein called H2-Ld SBM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	173	Total	C	N	O	S	0	0	0
			1436	900	255	274	7			
3	E	175	Total	C	N	O	S	0	0	0
			1449	907	258	277	7			
3	K	175	Total	C	N	O	S	0	0	0
			1448	908	257	276	7			
3	Q	176	Total	C	N	O	S	0	0	0
			1453	911	258	277	7			

- Molecule 4 is a protein called p5E8 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	9	Total	C	N	O	0	0	0
			85	62	10	13			
4	F	9	Total	C	N	O	0	0	0
			85	62	10	13			
4	L	9	Total	C	N	O	0	0	0
			85	62	10	13			
4	R	9	Total	C	N	O	0	0	0
			85	62	10	13			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

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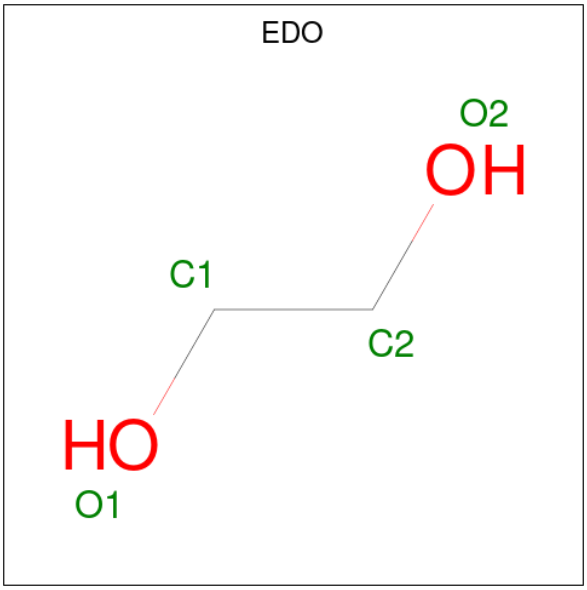
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0
5	N	1	Total O S 5 4 1	0	0
5	N	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	N	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

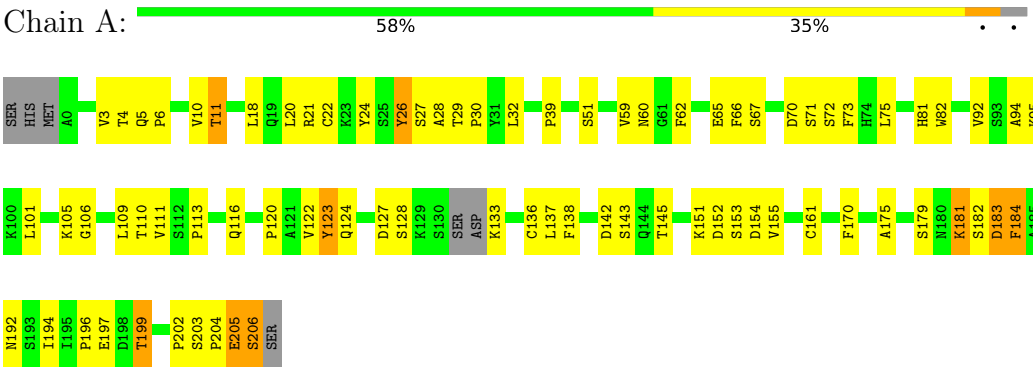
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total O 1 1	0	0
7	H	1	Total O 1 1	0	0
7	K	1	Total O 1 1	0	0
7	N	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

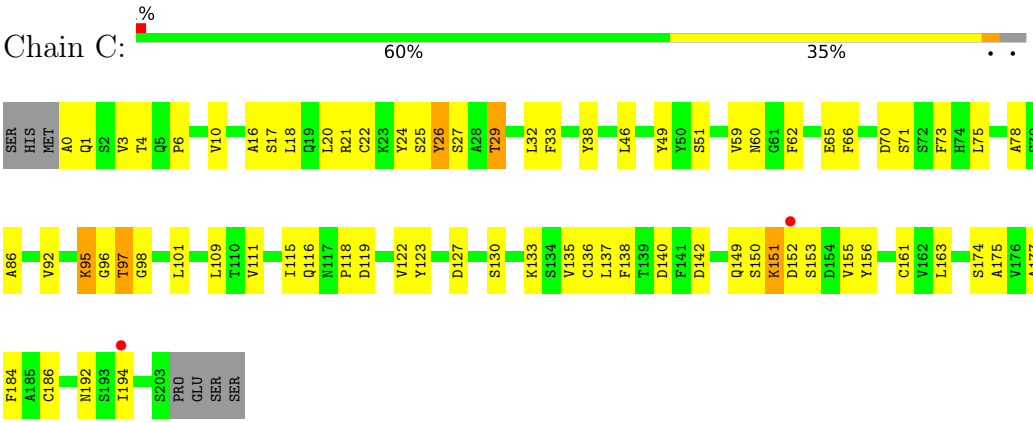
• Molecule 1: 42F3 alpha

Chain A:



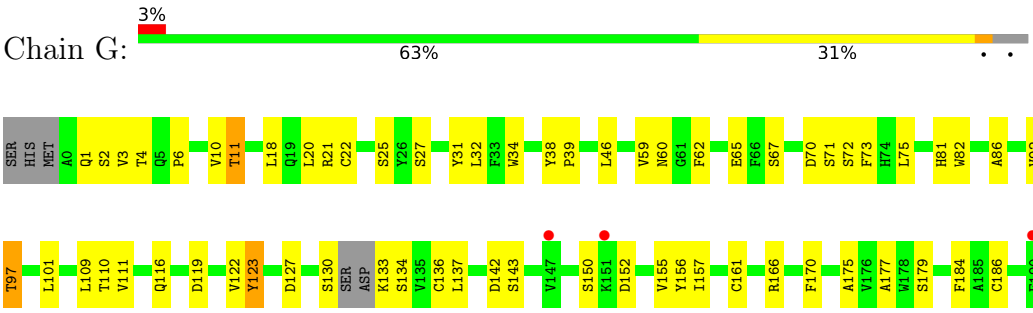
• Molecule 1: 42F3 alpha

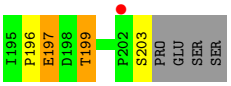
Chain C:



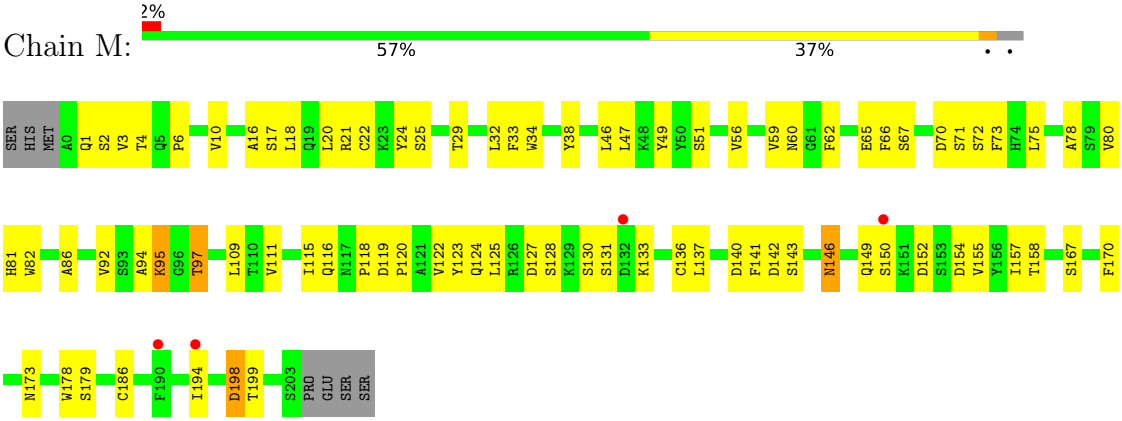
• Molecule 1: 42F3 alpha

Chain G:

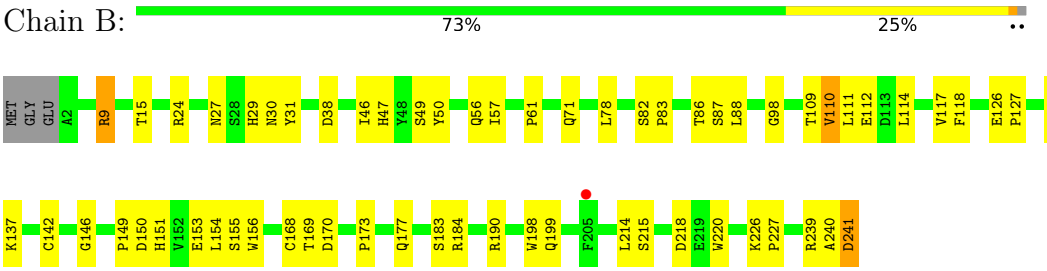




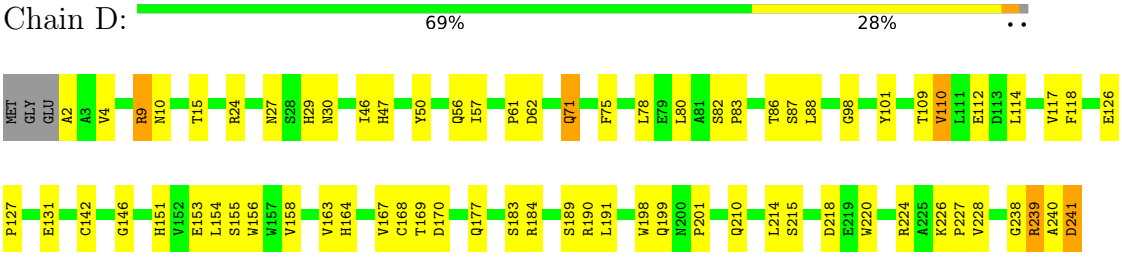
• Molecule 1: 42F3 alpha



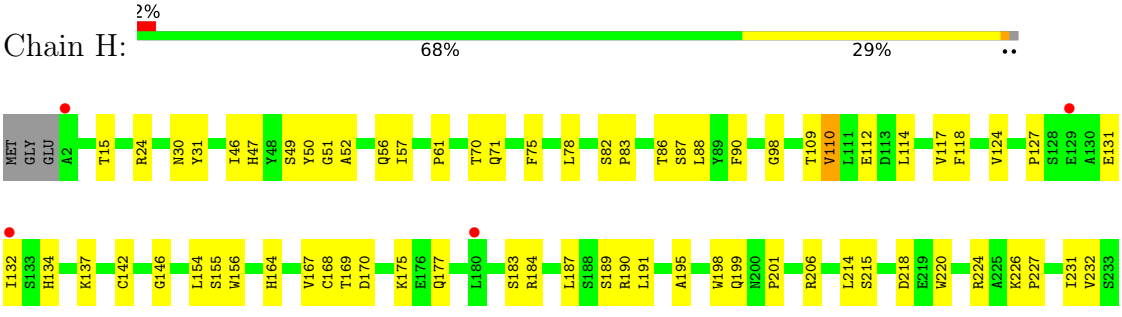
• Molecule 2: 42F3 beta

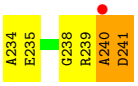


• Molecule 2: 42F3 beta



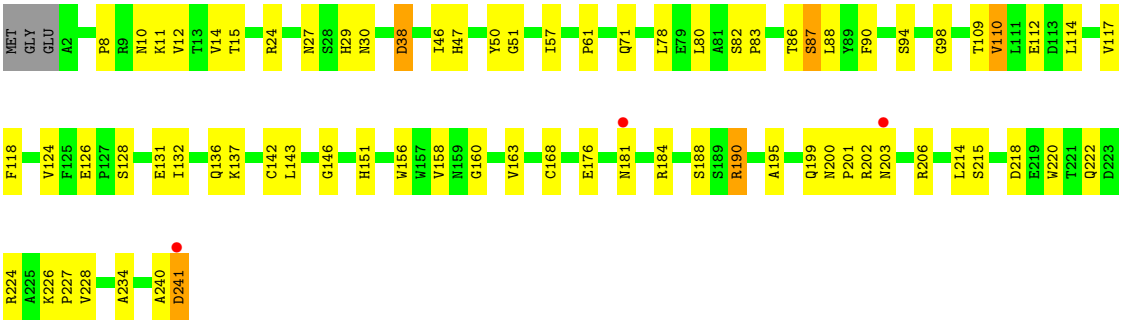
• Molecule 2: 42F3 beta





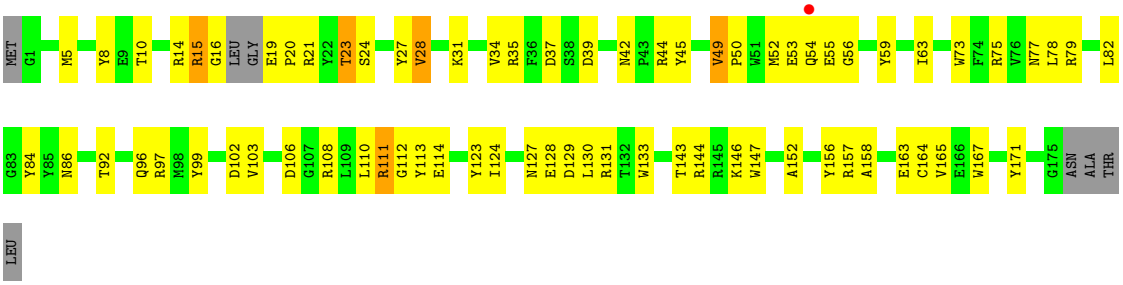
• Molecule 2: 42F3 beta

Chain N:



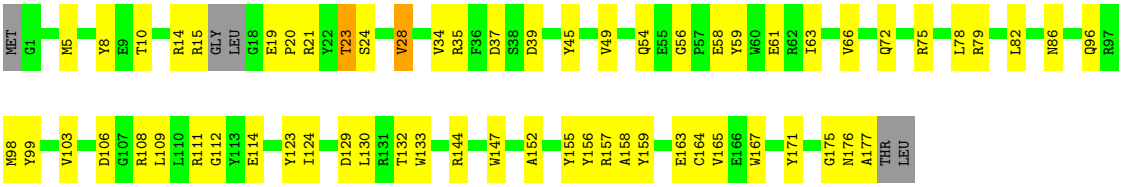
• Molecule 3: H2-Ld SBM2

Chain I:



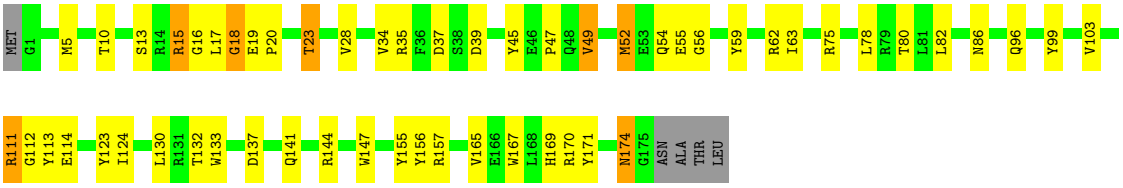
• Molecule 3: H2-Ld SBM2

Chain E:



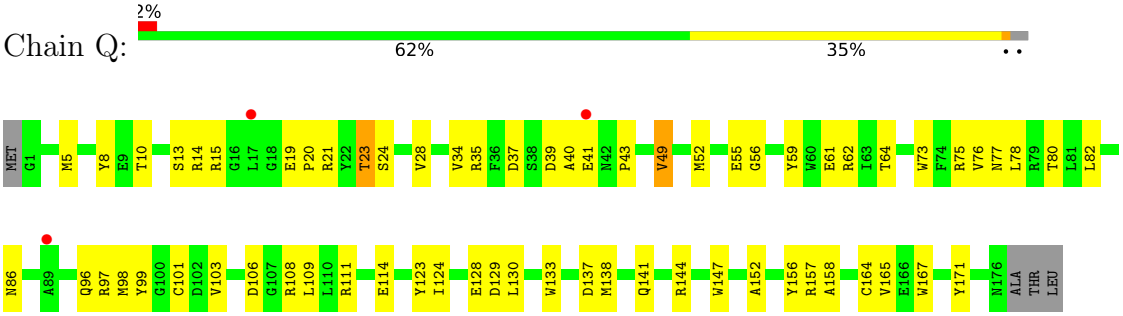
• Molecule 3: H2-Ld SBM2

Chain K:



• Molecule 3: H2-Ld SBM2

Chain Q:

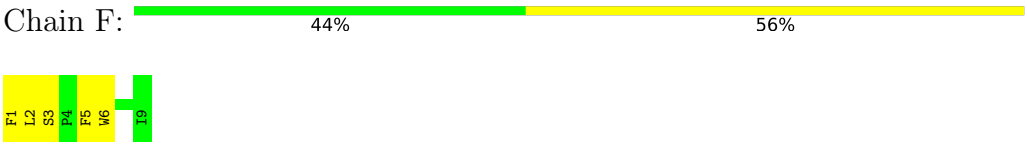


• Molecule 4: p5E8 peptide

Chain J:

• Molecule 4: p5E8 peptide

Chain F:

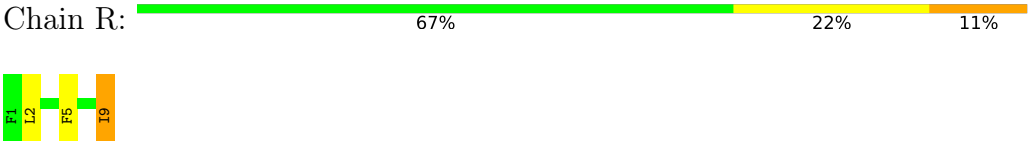


• Molecule 4: p5E8 peptide

Chain L:

• Molecule 4: p5E8 peptide

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	291.33Å 291.33Å 291.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.31 – 3.10 45.31 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.31-3.10) 99.6 (45.31-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.231 , 0.258 0.227 , 0.253	Depositor DCC
R_{free} test set	4272 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	67.0	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20148	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.59	0/1634	0.73	1/2214 (0.0%)
1	C	0.57	0/1623	0.73	1/2200 (0.0%)
1	G	0.64	0/1611	0.78	0/2182
1	M	0.58	0/1626	0.81	0/2204
2	B	0.61	0/1952	0.71	0/2662
2	D	0.58	0/1952	0.71	1/2662 (0.0%)
2	H	0.59	0/1952	0.74	2/2662 (0.1%)
2	N	0.62	1/1952 (0.1%)	0.73	1/2662 (0.0%)
3	E	0.59	1/1488 (0.1%)	0.70	0/2014
3	I	0.59	0/1475	0.69	0/1996
3	K	0.69	0/1488	0.73	1/2015 (0.0%)
3	Q	0.57	0/1493	0.74	0/2022
4	F	0.66	0/90	0.60	0/121
4	J	0.68	0/90	0.67	0/121
4	L	0.82	0/90	0.70	0/121
4	R	1.02	0/90	0.76	0/121
All	All	0.61	2/20606 (0.0%)	0.73	7/27979 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	8	PRO	N-CD	-5.60	1.40	1.47
3	E	72	GLN	CD-OE1	5.33	1.35	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	VAL	N-CA-C	-6.27	94.07	111.00
2	H	240	ALA	N-CA-CB	5.88	118.33	110.10
2	N	203	ASN	N-CA-C	5.68	126.35	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	18	GLY	N-CA-C	-5.34	99.74	113.10
1	C	142	ASP	N-CA-C	5.21	125.07	111.00
2	H	235	GLU	N-CA-C	5.14	124.89	111.00
1	A	181	LYS	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1595	0	1523	78	0
1	C	1584	0	1509	70	0
1	G	1573	0	1505	58	0
1	M	1587	0	1515	67	1
2	B	1900	0	1797	57	0
2	D	1900	0	1797	72	0
2	H	1900	0	1797	69	0
2	N	1900	0	1796	67	1
3	E	1449	0	1333	56	0
3	I	1436	0	1322	73	0
3	K	1448	0	1339	48	0
3	Q	1453	0	1341	55	0
4	F	85	0	77	8	0
4	J	85	0	77	11	0
4	L	85	0	77	8	0
4	R	85	0	77	7	0
5	A	5	0	0	0	0
5	B	15	0	0	0	0
5	D	10	0	0	1	0
5	E	5	0	0	4	0
5	G	5	0	0	0	0
5	H	10	0	0	1	0
5	K	10	0	0	0	0
5	N	10	0	0	3	0
5	Q	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	4	0	6	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
7	K	1	0	0	0	0
7	N	1	0	0	0	0
All	All	20148	0	18888	735	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (735) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:CYS:HB3	2:B:168:CYS:SG	1.13	1.69
1:G:161:CYS:HB3	2:H:168:CYS:SG	1.34	1.63
1:C:161:CYS:HB3	2:D:168:CYS:SG	1.34	1.62
1:A:161:CYS:CB	2:B:168:CYS:SG	2.08	1.40
1:C:161:CYS:CB	2:D:168:CYS:SG	2.25	1.25
1:G:161:CYS:CB	2:H:168:CYS:SG	2.27	1.22
3:I:15:ARG:HD3	3:I:15:ARG:N	1.45	1.15
3:I:15:ARG:N	3:I:15:ARG:HH11	1.47	1.13
3:I:15:ARG:H	3:I:15:ARG:CD	1.60	1.11
2:D:239:ARG:HH11	2:D:239:ARG:CG	1.64	1.09
1:C:3:VAL:CG2	1:C:92:VAL:HG13	1.85	1.06
2:N:86:THR:HG23	2:N:109:THR:HA	1.38	1.05
3:I:15:ARG:HD3	3:I:15:ARG:H	0.88	1.05
2:D:239:ARG:HH11	2:D:239:ARG:HG3	1.16	1.05
1:M:67:SER:HB3	1:M:72:SER:HB3	1.35	1.03
1:G:197:GLU:OE1	1:G:197:GLU:HA	1.60	1.01
3:K:19:GLU:HG2	3:K:20:PRO:HD2	1.42	0.99
3:I:19:GLU:HG2	3:I:20:PRO:HD2	1.45	0.97
1:A:27:SER:O	1:A:30:PRO:HD3	1.64	0.97
3:Q:19:GLU:HG2	3:Q:20:PRO:HD2	1.46	0.97
1:M:142:ASP:OD1	1:M:143:SER:N	1.98	0.97
1:M:1:GLN:OE1	1:M:94:ALA:HA	1.63	0.97
3:E:19:GLU:HG2	3:E:20:PRO:HD2	1.48	0.96
3:E:129:ASP:OD1	3:E:132:THR:HG23	1.67	0.94
1:G:196:PRO:O	1:G:199:THR:HG23	1.70	0.92
3:E:5:MET:HE2	3:E:164:CYS:SG	2.10	0.91
4:L:1:PHE:HD1	4:L:1:PHE:O	1.53	0.91
1:A:161:CYS:HB3	2:B:168:CYS:HG	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:17:LEU:HD12	3:K:17:LEU:O	1.70	0.90
3:E:130:LEU:HB3	3:E:157:ARG:HG3	1.53	0.90
1:C:3:VAL:HG22	1:C:92:VAL:HG13	1.51	0.89
1:M:136:CYS:HG	1:M:186:CYS:HG	0.90	0.88
3:Q:130:LEU:HB3	3:Q:157:ARG:HG3	1.56	0.88
3:K:130:LEU:HB3	3:K:157:ARG:HG3	1.55	0.86
1:A:67:SER:HB3	1:A:72:SER:HB3	1.58	0.86
4:F:1:PHE:HD1	4:F:1:PHE:O	1.59	0.85
4:F:1:PHE:O	4:F:1:PHE:CD1	2.30	0.84
3:E:5:MET:CE	3:E:164:CYS:SG	2.65	0.84
1:A:136:CYS:HG	1:A:186:CYS:HG	0.85	0.84
1:C:16:ALA:O	1:C:80:VAL:HG22	1.76	0.84
4:L:1:PHE:O	4:L:1:PHE:CD1	2.30	0.84
2:N:160:GLY:HA2	5:N:243:SO4:O3	1.79	0.83
2:D:239:ARG:HG3	2:D:239:ARG:NH1	1.89	0.83
3:I:111:ARG:NH1	3:I:128:GLU:HB2	1.94	0.83
3:E:130:LEU:HD23	3:E:157:ARG:HG2	1.60	0.83
1:A:161:CYS:CB	2:B:168:CYS:HG	1.86	0.83
3:I:123:TYR:HD1	3:I:124:ILE:HG22	1.44	0.83
2:D:239:ARG:CG	2:D:239:ARG:NH1	2.37	0.82
3:Q:123:TYR:HD1	3:Q:124:ILE:HG22	1.44	0.82
3:I:15:ARG:N	3:I:15:ARG:CD	2.29	0.82
3:I:52:MET:O	3:I:55:GLU:HG3	1.77	0.82
3:I:130:LEU:HB3	3:I:157:ARG:HG3	1.62	0.81
2:N:88:LEU:HD21	2:N:90:PHE:CZ	2.15	0.81
2:H:50:TYR:HE2	2:H:56:GLN:HG3	1.45	0.80
1:G:101:LEU:HD13	2:H:98:GLY:HA2	1.64	0.79
1:A:194:ILE:O	1:A:194:ILE:HG22	1.83	0.79
2:D:83:PRO:HA	2:D:110:VAL:HG22	1.64	0.79
2:H:86:THR:HG23	2:H:109:THR:HA	1.63	0.79
1:M:51:SER:HB3	3:Q:158:ALA:HB2	1.63	0.78
3:I:14:ARG:HB3	3:I:15:ARG:NH1	1.98	0.78
1:M:3:VAL:CG2	1:M:22:CYS:SG	2.72	0.78
3:E:123:TYR:HD1	3:E:124:ILE:HG22	1.47	0.78
3:Q:101:CYS:CB	3:Q:164:CYS:HG	1.97	0.77
3:Q:52:MET:O	3:Q:55:GLU:HG3	1.84	0.77
3:K:52:MET:O	3:K:55:GLU:HG3	1.85	0.77
1:M:81:HIS:O	1:M:111:VAL:HG11	1.83	0.77
2:D:75:PHE:CG	2:N:80:LEU:HD13	2.20	0.76
1:G:67:SER:HB3	1:G:72:SER:HB3	1.66	0.76
3:I:5:MET:HE2	3:I:164:CYS:SG	2.26	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:15:ARG:N	3:I:15:ARG:NH1	2.30	0.76
3:I:15:ARG:H	3:I:15:ARG:NH1	1.83	0.76
2:H:78:LEU:N	2:H:78:LEU:HD12	2.01	0.75
2:H:46:ILE:HG22	2:H:47:HIS:CD2	2.21	0.75
3:K:111:ARG:HG3	3:K:112:GLY:N	2.02	0.75
1:A:3:VAL:CG2	1:A:22:CYS:SG	2.75	0.74
1:G:3:VAL:CG2	1:G:22:CYS:SG	2.75	0.74
3:Q:49:VAL:HG12	3:Q:52:MET:HG2	1.69	0.74
1:G:1:GLN:NE2	1:G:27:SER:HB2	2.02	0.74
2:B:111:LEU:HD21	2:B:149:PRO:HG3	1.69	0.74
1:M:194:ILE:O	1:M:194:ILE:HG22	1.87	0.74
3:Q:101:CYS:CB	3:Q:164:CYS:SG	2.76	0.73
3:I:111:ARG:HH11	3:I:128:GLU:HB2	1.51	0.73
2:H:88:LEU:HD21	2:H:90:PHE:CZ	2.24	0.73
3:K:54:GLN:O	3:K:54:GLN:HG3	1.87	0.73
2:H:117:VAL:HG12	2:H:227:PRO:HB2	1.69	0.73
3:I:5:MET:CE	3:I:164:CYS:SG	2.77	0.72
2:N:195:ALA:O	2:N:199:GLN:HG3	1.88	0.72
2:N:117:VAL:HG12	2:N:227:PRO:HB2	1.70	0.72
2:D:27:ASN:HB3	2:D:29:HIS:CD2	2.25	0.72
3:E:75:ARG:NH2	5:E:180:SO4:O2	2.23	0.71
2:D:214:LEU:HD13	2:D:227:PRO:HG2	1.70	0.71
3:E:37:ASP:OD1	3:E:39:ASP:HB2	1.89	0.71
3:I:37:ASP:OD1	3:I:39:ASP:HB2	1.91	0.71
1:A:151:LYS:CD	1:A:192:ASN:OD1	2.39	0.71
2:D:199:GLN:HA	2:D:239:ARG:O	1.89	0.71
2:D:117:VAL:O	2:D:224:ARG:NH2	2.23	0.71
3:Q:103:VAL:HG11	3:Q:165:VAL:HG13	1.72	0.71
1:C:183:ASP:OD1	1:C:183:ASP:C	2.30	0.70
1:A:124:GLN:HB2	1:A:186:CYS:SG	2.31	0.70
2:D:78:LEU:N	2:D:78:LEU:HD12	2.06	0.70
3:Q:101:CYS:HB3	3:Q:164:CYS:SG	2.31	0.70
2:D:46:ILE:HG22	2:D:47:HIS:CD2	2.26	0.70
1:C:151:LYS:HG3	1:C:152:ASP:N	2.06	0.70
2:H:156:TRP:HD1	2:H:167:VAL:HG11	1.56	0.70
1:C:136:CYS:SG	1:C:184:PHE:CE2	2.85	0.70
1:C:3:VAL:HG22	1:C:92:VAL:CG1	2.20	0.69
2:B:86:THR:HG23	2:B:109:THR:HA	1.75	0.69
3:E:103:VAL:HG11	3:E:165:VAL:HG13	1.72	0.69
2:N:88:LEU:HD23	2:N:90:PHE:CE2	2.27	0.69
1:A:183:ASP:O	1:A:184:PHE:CB	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:ILE:HG22	1:G:194:ILE:O	1.93	0.69
3:E:176:ASN:O	3:E:177:ALA:O	2.10	0.69
2:B:46:ILE:HG22	2:B:47:HIS:CD2	2.26	0.69
1:C:194:ILE:O	1:C:194:ILE:HG22	1.93	0.69
1:G:81:HIS:O	1:G:111:VAL:HG11	1.93	0.69
2:N:200:ASN:OD1	2:N:201:PRO:HD2	1.92	0.69
1:C:6:PRO:HG3	1:C:21:ARG:HB2	1.74	0.69
2:H:50:TYR:CE2	2:H:56:GLN:HG3	2.28	0.69
1:C:161:CYS:HB3	2:D:168:CYS:HG	1.54	0.69
3:I:103:VAL:HG11	3:I:165:VAL:HG13	1.75	0.68
1:M:123:TYR:CE1	2:N:131:GLU:HA	2.27	0.68
1:A:183:ASP:OD1	1:A:183:ASP:C	2.30	0.68
3:E:10:THR:HG22	3:E:96:GLN:HG3	1.75	0.68
2:D:2:ALA:HB2	2:D:101:TYR:HD1	1.58	0.68
3:I:15:ARG:HH11	3:I:15:ARG:H	1.15	0.68
2:D:82:SER:C	2:D:110:VAL:HG21	2.14	0.68
1:M:3:VAL:HG21	1:M:22:CYS:SG	2.33	0.68
3:Q:130:LEU:HB3	3:Q:157:ARG:CG	2.24	0.68
1:A:3:VAL:HG21	1:A:22:CYS:SG	2.34	0.68
2:H:156:TRP:CD1	2:H:167:VAL:HG11	2.28	0.67
2:H:117:VAL:O	2:H:224:ARG:NH2	2.28	0.67
2:D:117:VAL:HG12	2:D:227:PRO:HB2	1.76	0.67
1:A:81:HIS:O	1:A:111:VAL:HG11	1.94	0.67
2:B:78:LEU:N	2:B:78:LEU:HD12	2.10	0.67
3:Q:37:ASP:OD1	3:Q:39:ASP:HB2	1.93	0.67
4:L:1:PHE:CD1	4:L:1:PHE:C	2.68	0.67
2:D:83:PRO:HA	2:D:110:VAL:CG2	2.23	0.67
3:K:37:ASP:OD1	3:K:39:ASP:HB2	1.95	0.67
1:M:124:GLN:HB2	1:M:186:CYS:SG	2.35	0.67
2:D:146:GLY:O	2:D:184:ARG:HD2	1.95	0.66
1:G:3:VAL:HG21	1:G:22:CYS:SG	2.36	0.66
1:M:6:PRO:HG3	1:M:21:ARG:HB2	1.76	0.66
3:I:129:ASP:O	3:I:131:ARG:NH1	2.27	0.66
3:E:54:GLN:O	3:E:54:GLN:HG2	1.95	0.66
1:A:6:PRO:HG3	1:A:21:ARG:HB2	1.78	0.66
3:K:123:TYR:HD1	3:K:124:ILE:HG22	1.59	0.66
1:G:142:ASP:OD2	1:G:142:ASP:C	2.33	0.66
2:H:214:LEU:HD13	2:H:227:PRO:HG2	1.78	0.65
2:N:46:ILE:HG22	2:N:47:HIS:CD2	2.30	0.65
2:N:214:LEU:HD13	2:N:227:PRO:HG2	1.77	0.65
1:A:183:ASP:OD1	1:A:184:PHE:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:88:LEU:CD2	2:H:90:PHE:CE2	2.79	0.65
3:K:103:VAL:HG11	3:K:165:VAL:HG13	1.79	0.65
2:D:239:ARG:HD3	2:D:241:ASP:OD2	1.96	0.65
2:H:156:TRP:CD1	2:H:167:VAL:CG1	2.80	0.65
3:Q:128:GLU:O	3:Q:130:LEU:HD13	1.97	0.65
1:A:5:GLN:O	1:A:105:LYS:HE3	1.97	0.65
2:D:239:ARG:HH11	2:D:239:ARG:HG2	1.58	0.65
3:E:129:ASP:OD1	3:E:132:THR:CG2	2.43	0.65
3:Q:101:CYS:HG	3:Q:164:CYS:HG	0.66	0.65
1:G:136:CYS:SG	1:G:186:CYS:HA	2.37	0.64
1:A:51:SER:HB3	3:I:158:ALA:HB2	1.79	0.64
2:B:87:SER:OG	2:B:88:LEU:N	2.30	0.64
3:I:123:TYR:CD1	3:I:124:ILE:HG22	2.31	0.64
3:E:130:LEU:HB3	3:E:157:ARG:CG	2.27	0.64
2:N:87:SER:OG	2:N:88:LEU:N	2.30	0.64
2:N:88:LEU:CD2	2:N:90:PHE:CE2	2.80	0.64
3:K:10:THR:HG22	3:K:96:GLN:HG3	1.79	0.64
2:H:88:LEU:HD23	2:H:90:PHE:CE2	2.32	0.64
1:M:146:ASN:OD1	1:M:146:ASN:N	2.30	0.63
3:K:130:LEU:HB3	3:K:157:ARG:CG	2.27	0.63
3:E:123:TYR:CD1	3:E:124:ILE:HG22	2.31	0.63
2:B:146:GLY:O	2:B:184:ARG:HD2	1.98	0.63
2:H:24:ARG:HG3	2:H:24:ARG:HH11	1.64	0.63
3:Q:123:TYR:CD1	3:Q:124:ILE:HG22	2.29	0.63
1:A:202:PRO:O	1:A:206:SER:N	2.29	0.63
2:H:146:GLY:O	2:H:184:ARG:HD2	1.99	0.63
2:H:164:HIS:O	2:H:167:VAL:HG23	1.98	0.63
3:I:10:THR:HG22	3:I:96:GLN:HG3	1.80	0.63
3:I:15:ARG:HD2	3:I:92:THR:OG1	1.99	0.63
1:C:32:LEU:CD2	1:C:92:VAL:HG12	2.28	0.62
2:D:118:PHE:CD2	2:D:184:ARG:HD3	2.33	0.62
3:I:5:MET:SD	3:I:167:TRP:CE3	2.93	0.62
3:K:16:GLY:H	3:K:17:LEU:HA	1.64	0.62
3:E:5:MET:SD	3:E:167:TRP:CE3	2.92	0.62
1:A:181:LYS:HB2	1:A:183:ASP:O	2.00	0.62
2:B:47:HIS:CE1	2:B:61:PRO:CB	2.82	0.62
2:D:47:HIS:ND1	2:D:57:ILE:HA	2.15	0.62
2:H:47:HIS:CE1	2:H:61:PRO:CB	2.83	0.62
2:H:118:PHE:CD2	2:H:184:ARG:HD3	2.33	0.62
3:E:79:ARG:NH1	5:E:180:SO4:O4	2.26	0.62
1:M:38:TYR:CD1	1:M:86:ALA:HB2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:99:TYR:HB3	3:I:114:GLU:OE2	1.99	0.62
1:G:6:PRO:HG3	1:G:21:ARG:HB2	1.81	0.62
3:K:156:TYR:OH	4:L:5:PHE:HA	2.00	0.62
3:Q:10:THR:HG22	3:Q:96:GLN:HG3	1.80	0.62
1:A:183:ASP:O	1:A:184:PHE:HB3	1.99	0.62
1:C:29:THR:HG23	3:E:163:GLU:OE2	2.00	0.62
3:E:75:ARG:NE	5:E:180:SO4:O2	2.32	0.61
2:H:177:GLN:O	2:H:183:SER:HB2	2.00	0.61
3:K:59:TYR:CD1	3:K:62:ARG:NH2	2.68	0.61
2:N:88:LEU:CD2	2:N:90:PHE:CZ	2.83	0.61
1:G:127:ASP:HB2	1:G:133:LYS:HB2	1.83	0.61
1:M:38:TYR:HD1	1:M:86:ALA:HB2	1.65	0.61
3:I:106:ASP:OD2	3:I:108:ARG:HG3	2.00	0.61
2:N:47:HIS:CE1	2:N:61:PRO:CB	2.84	0.61
2:B:214:LEU:HD13	2:B:227:PRO:HG2	1.82	0.61
3:E:99:TYR:HB3	3:E:114:GLU:OE2	2.01	0.60
3:K:59:TYR:CE1	3:K:62:ARG:NH2	2.68	0.60
3:K:80:THR:HG21	4:L:9:ILE:HG22	1.83	0.60
3:I:131:ARG:HG3	3:I:131:ARG:HH11	1.66	0.60
3:I:146:LYS:HD2	4:J:9:ILE:OXT	2.01	0.60
2:H:88:LEU:HD23	2:H:90:PHE:HE2	1.65	0.60
1:G:122:VAL:HG12	1:G:122:VAL:O	1.99	0.60
1:M:32:LEU:CD2	1:M:92:VAL:HG12	2.32	0.60
2:N:47:HIS:ND1	2:N:57:ILE:HA	2.16	0.60
2:H:47:HIS:CE1	2:H:61:PRO:HB3	2.37	0.60
2:N:78:LEU:N	2:N:78:LEU:HD12	2.17	0.60
2:H:47:HIS:ND1	2:H:57:ILE:HA	2.16	0.60
2:D:24:ARG:HG3	2:D:24:ARG:HH11	1.67	0.60
3:Q:137:ASP:O	3:Q:141:GLN:HG2	2.02	0.60
1:A:123:TYR:CE1	2:B:131:GLU:HA	2.37	0.59
1:G:70:ASP:HB3	1:G:72:SER:HB2	1.84	0.59
2:N:88:LEU:HD23	2:N:90:PHE:HE2	1.66	0.59
1:A:170:PHE:CE2	2:B:137:LYS:HE3	2.38	0.59
2:B:47:HIS:CE1	2:B:61:PRO:HB3	2.37	0.59
3:I:130:LEU:HB3	3:I:157:ARG:CG	2.31	0.59
3:I:75:ARG:NH1	3:I:79:ARG:HH12	2.00	0.59
2:H:82:SER:C	2:H:110:VAL:HG21	2.23	0.59
2:D:50:TYR:HE2	2:D:56:GLN:HG3	1.68	0.59
3:K:141:GLN:OE1	3:K:144:ARG:NH2	2.35	0.59
1:M:178:TRP:CD2	2:N:143:LEU:HD21	2.38	0.59
2:H:154:LEU:HD23	2:H:155:SER:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:28:VAL:HG21	3:E:171:TYR:CE2	2.38	0.59
3:Q:99:TYR:HB3	3:Q:114:GLU:OE2	2.03	0.59
1:M:70:ASP:HB3	1:M:72:SER:HB2	1.84	0.58
2:N:82:SER:C	2:N:110:VAL:HG21	2.24	0.58
1:A:70:ASP:HB3	1:A:72:SER:HB2	1.85	0.58
1:A:32:LEU:CD2	1:A:92:VAL:HG12	2.33	0.58
1:A:95:LYS:NZ	4:J:1:PHE:CE2	2.62	0.58
2:D:86:THR:HG23	2:D:109:THR:HA	1.85	0.58
1:A:194:ILE:O	1:A:194:ILE:CG2	2.51	0.58
1:C:149:GLN:HG3	1:C:150:SER:N	2.19	0.58
2:N:222:GLN:HG2	2:N:224:ARG:NH1	2.19	0.58
1:A:94:ALA:HB3	1:A:97:THR:HB	1.86	0.58
3:E:21:ARG:NE	3:E:39:ASP:OD2	2.37	0.58
4:F:1:PHE:CD1	4:F:1:PHE:C	2.77	0.58
2:B:215:SER:HB3	2:B:218:ASP:OD1	2.03	0.57
3:E:34:VAL:HG22	3:E:35:ARG:N	2.18	0.57
2:B:82:SER:C	2:B:110:VAL:HG21	2.25	0.57
3:I:28:VAL:HG21	3:I:171:TYR:CE2	2.40	0.57
1:G:150:SER:HB3	1:G:157:ILE:HD12	1.84	0.57
1:C:17:SER:HA	1:C:78:ALA:O	2.04	0.57
1:C:24:TYR:HH	1:C:66:PHE:HE1	1.51	0.57
2:N:118:PHE:CD2	2:N:184:ARG:HD3	2.40	0.57
1:G:32:LEU:CD2	1:G:92:VAL:HG12	2.35	0.57
3:Q:156:TYR:OH	4:R:5:PHE:HA	2.05	0.57
2:B:30:ASN:HB3	2:B:50:TYR:O	2.04	0.57
2:D:10:ASN:OD1	2:D:151:HIS:NE2	2.28	0.57
3:E:176:ASN:O	3:E:177:ALA:C	2.42	0.57
3:I:133:TRP:HB2	3:I:144:ARG:HG3	1.87	0.57
1:M:1:GLN:OE1	1:M:94:ALA:CA	2.46	0.56
3:Q:34:VAL:HG22	3:Q:35:ARG:N	2.20	0.56
3:E:19:GLU:HG3	3:E:75:ARG:HH11	1.70	0.56
1:M:155:VAL:HG22	1:M:179:SER:HB2	1.86	0.56
1:M:82:TRP:HD1	1:M:111:VAL:O	1.89	0.56
1:M:120:PRO:HB2	1:M:199:THR:HA	1.87	0.56
3:Q:21:ARG:NE	3:Q:39:ASP:OD2	2.37	0.56
1:A:120:PRO:HB2	1:A:199:THR:HB	1.87	0.56
3:E:156:TYR:OH	4:F:5:PHE:HA	2.06	0.56
3:I:73:TRP:CE2	3:I:77:ASN:ND2	2.74	0.56
2:H:83:PRO:HA	2:H:110:VAL:CG2	2.36	0.56
1:M:115:ILE:HG22	1:M:118:PRO:HD3	1.87	0.56
2:D:9:ARG:NH1	2:D:153:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:14:ARG:HD2	3:Q:19:GLU:O	2.05	0.56
1:A:95:LYS:NZ	3:I:163:GLU:OE1	2.39	0.55
2:B:50:TYR:HE2	2:B:56:GLN:HG3	1.71	0.55
1:C:136:CYS:SG	1:C:184:PHE:CZ	2.99	0.55
1:G:123:TYR:CE1	2:H:131:GLU:HA	2.41	0.55
1:G:127:ASP:HB3	1:G:130:SER:O	2.06	0.55
3:K:137:ASP:O	3:K:141:GLN:HG2	2.06	0.55
1:M:70:ASP:CB	1:M:72:SER:HB2	2.37	0.55
2:N:14:VAL:HG22	2:N:114:LEU:HD21	1.88	0.55
2:D:47:HIS:CE1	2:D:61:PRO:CB	2.90	0.55
2:N:201:PRO:CD	2:N:202:ARG:H	2.20	0.55
3:Q:28:VAL:HG21	3:Q:171:TYR:CE2	2.41	0.55
3:I:84:TYR:HE2	4:J:9:ILE:HG22	1.71	0.55
2:H:215:SER:HB3	2:H:218:ASP:OD1	2.07	0.55
1:G:127:ASP:OD2	1:G:133:LYS:HD3	2.07	0.55
1:M:2:SER:H	1:M:25:SER:HB2	1.72	0.55
2:N:47:HIS:CE1	2:N:61:PRO:HB3	2.41	0.55
1:G:197:GLU:OE1	1:G:197:GLU:CA	2.42	0.55
1:A:181:LYS:CB	1:A:183:ASP:O	2.56	0.54
1:C:32:LEU:HD23	1:C:92:VAL:HG12	1.89	0.54
1:G:137:LEU:HD12	1:G:175:ALA:O	2.06	0.54
1:A:161:CYS:SG	2:B:168:CYS:SG	3.06	0.54
1:M:122:VAL:HG12	1:M:122:VAL:O	2.07	0.54
3:I:21:ARG:NE	3:I:39:ASP:OD2	2.38	0.54
1:C:95:LYS:NZ	4:F:3:SER:HA	2.23	0.54
1:M:194:ILE:O	1:M:194:ILE:CG2	2.54	0.54
3:Q:106:ASP:OD2	3:Q:108:ARG:HG3	2.07	0.54
1:A:59:VAL:HG22	1:A:60:ASN:N	2.23	0.54
2:D:87:SER:OG	2:D:88:LEU:N	2.41	0.54
1:G:59:VAL:HG22	1:G:60:ASN:N	2.22	0.54
3:Q:109:LEU:HD11	3:Q:111:ARG:O	2.07	0.54
3:I:143:THR:HA	4:J:9:ILE:OXT	2.08	0.54
2:H:24:ARG:HG3	2:H:24:ARG:NH1	2.22	0.54
1:A:11:THR:HG23	1:A:110:THR:HB	1.91	0.53
3:E:75:ARG:CZ	5:E:180:SO4:O2	2.57	0.53
1:A:152:ASP:O	1:A:154:ASP:N	2.34	0.53
1:A:203:SER:N	1:A:204:PRO:HD2	2.23	0.53
3:K:59:TYR:HD1	3:K:62:ARG:HH22	1.57	0.53
3:E:15:ARG:NH1	3:Q:61:GLU:HB2	2.24	0.53
3:I:102:ASP:O	3:I:110:LEU:HB3	2.08	0.53
2:D:78:LEU:N	2:D:78:LEU:CD1	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2:SER:H	1:M:25:SER:CB	2.20	0.53
3:K:99:TYR:HB3	3:K:114:GLU:OE2	2.09	0.53
3:K:130:LEU:HD23	3:K:157:ARG:HG2	1.91	0.53
3:I:34:VAL:HG22	3:I:35:ARG:N	2.24	0.53
2:D:215:SER:HB3	2:D:218:ASP:OD1	2.07	0.53
3:E:109:LEU:HD11	3:E:111:ARG:O	2.09	0.53
1:G:196:PRO:O	1:G:199:THR:CG2	2.51	0.53
1:A:32:LEU:HD13	1:A:73:PHE:HB2	1.91	0.53
3:I:49:VAL:O	3:I:53:GLU:HG3	2.09	0.53
2:D:167:VAL:HG22	2:D:191:LEU:HD13	1.91	0.53
2:D:177:GLN:O	2:D:183:SER:HB2	2.09	0.53
2:N:160:GLY:CA	5:N:243:SO4:O3	2.55	0.53
2:D:47:HIS:CE1	2:D:61:PRO:HB3	2.44	0.53
3:I:14:ARG:HB3	3:I:15:ARG:HH12	1.74	0.52
2:N:88:LEU:HD21	2:N:90:PHE:HZ	1.70	0.52
3:Q:19:GLU:HG3	3:Q:75:ARG:HH11	1.74	0.52
3:I:130:LEU:CD1	3:I:130:LEU:N	2.71	0.52
3:E:106:ASP:OD2	3:E:108:ARG:HG3	2.09	0.52
2:N:83:PRO:HA	2:N:110:VAL:HG22	1.91	0.52
1:M:136:CYS:SG	1:M:186:CYS:HA	2.49	0.52
2:N:27:ASN:HB3	2:N:29:HIS:CD2	2.44	0.52
3:E:14:ARG:HD2	3:E:19:GLU:O	2.09	0.52
1:G:155:VAL:HG22	1:G:179:SER:HB2	1.89	0.52
4:J:9:ILE:HG22	4:J:9:ILE:O	2.10	0.52
2:D:142:CYS:HB2	2:D:156:TRP:CH2	2.44	0.52
2:H:46:ILE:HG22	2:H:47:HIS:HD2	1.73	0.52
3:K:111:ARG:HG2	3:K:113:TYR:CZ	2.45	0.52
3:K:34:VAL:HG22	3:K:35:ARG:N	2.24	0.52
2:N:15:THR:HG23	2:N:83:PRO:HD3	1.90	0.52
2:N:215:SER:HB3	2:N:218:ASP:OD1	2.09	0.52
1:G:82:TRP:HD1	1:G:111:VAL:O	1.92	0.52
2:H:51:GLY:O	2:H:52:ALA:C	2.47	0.52
3:K:132:THR:HG22	3:K:133:TRP:N	2.25	0.52
2:N:146:GLY:O	2:N:184:ARG:HD2	2.10	0.52
2:N:206:ARG:NH2	5:N:243:SO4:O2	2.42	0.52
2:D:2:ALA:HB2	2:D:101:TYR:CD1	2.43	0.52
2:D:50:TYR:CE2	2:D:56:GLN:HG3	2.44	0.52
2:B:24:ARG:HG3	2:B:24:ARG:HH11	1.74	0.51
2:B:150:ASP:OD1	2:B:150:ASP:C	2.47	0.51
1:M:127:ASP:HB3	1:M:130:SER:O	2.10	0.51
2:N:11:LYS:HG3	2:N:12:VAL:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:THR:HG23	2:B:83:PRO:HD3	1.91	0.51
1:M:32:LEU:HD13	1:M:73:PHE:HB2	1.92	0.51
1:C:82:TRP:HD1	1:C:111:VAL:O	1.93	0.51
1:M:119:ASP:O	1:M:140:ASP:HB2	2.11	0.51
3:I:131:ARG:NH1	3:I:131:ARG:HG3	2.25	0.51
1:M:18:LEU:HD11	1:M:20:LEU:HG	1.92	0.51
2:N:30:ASN:HB3	2:N:50:TYR:O	2.10	0.51
3:I:5:MET:SD	3:I:167:TRP:HE3	2.33	0.51
1:C:3:VAL:HG23	1:C:92:VAL:HG13	1.88	0.51
3:E:111:ARG:HG3	3:E:112:GLY:H	1.75	0.51
2:H:117:VAL:HG11	2:H:214:LEU:CD1	2.40	0.51
2:B:149:PRO:O	2:B:151:HIS:N	2.44	0.51
3:E:111:ARG:HG3	3:E:112:GLY:N	2.25	0.51
3:E:129:ASP:O	3:E:130:LEU:HB2	2.11	0.51
3:K:17:LEU:HD11	3:K:75:ARG:HH21	1.76	0.51
2:D:2:ALA:HB1	2:D:101:TYR:HB3	1.93	0.51
3:Q:130:LEU:HD12	3:Q:130:LEU:N	2.25	0.51
1:C:137:LEU:HD11	1:C:174:SER:OG	2.11	0.51
2:B:27:ASN:HB3	2:B:29:HIS:CD2	2.46	0.51
3:I:111:ARG:HG3	3:I:112:GLY:N	2.25	0.51
3:E:5:MET:SD	3:E:167:TRP:HE3	2.34	0.51
3:E:133:TRP:HB2	3:E:144:ARG:HG3	1.92	0.51
1:A:120:PRO:HB2	1:A:199:THR:HA	1.93	0.50
1:A:151:LYS:HD3	1:A:192:ASN:OD1	2.10	0.50
1:C:136:CYS:SG	1:C:184:PHE:HE2	2.33	0.50
1:M:158:THR:HG21	2:N:188:SER:OG	2.12	0.50
3:K:147:TRP:NE1	4:L:8:ASP:O	2.38	0.50
1:C:98:GLY:HA3	4:F:6:TRP:NE1	2.26	0.50
2:H:199:GLN:HA	2:H:239:ARG:O	2.12	0.50
1:C:101:LEU:HD13	2:D:98:GLY:HA2	1.93	0.50
2:H:134:HIS:HD2	2:H:134:HIS:O	1.94	0.50
4:J:1:PHE:CG	4:J:2:LEU:N	2.80	0.50
1:G:150:SER:HB3	1:G:157:ILE:CD1	2.40	0.50
2:H:83:PRO:HA	2:H:110:VAL:HG22	1.94	0.50
2:B:114:LEU:HD22	2:B:214:LEU:HD21	1.93	0.50
2:B:150:ASP:OD1	2:B:150:ASP:O	2.30	0.50
3:I:15:ARG:NH1	3:I:16:GLY:H	2.09	0.50
2:H:78:LEU:N	2:H:78:LEU:CD1	2.70	0.50
2:H:82:SER:O	2:H:110:VAL:HG21	2.12	0.50
1:M:198:ASP:C	1:M:198:ASP:OD2	2.50	0.50
2:B:83:PRO:HA	2:B:110:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:HD13	1:C:73:PHE:HB2	1.93	0.50
2:B:114:LEU:HD13	2:B:214:LEU:CD2	2.43	0.49
3:K:19:GLU:CG	3:K:20:PRO:HD2	2.30	0.49
1:M:24:TYR:HH	1:M:66:PHE:HE1	1.59	0.49
1:M:82:TRP:HA	1:M:111:VAL:CG1	2.41	0.49
1:A:26:TYR:C	1:A:26:TYR:CD2	2.81	0.49
1:A:70:ASP:O	1:A:71:SER:HB2	2.11	0.49
1:G:1:GLN:NE2	1:G:27:SER:CB	2.73	0.49
2:H:206:ARG:NE	5:H:243:SO4:O3	2.44	0.49
3:K:56:GLY:O	3:K:59:TYR:HB3	2.13	0.49
1:M:150:SER:HB3	1:M:157:ILE:CD1	2.43	0.49
2:N:38:ASP:OD1	2:N:87:SER:HB2	2.12	0.49
2:B:118:PHE:CD2	2:B:184:ARG:HD3	2.48	0.49
2:B:240:ALA:O	2:B:241:ASP:C	2.51	0.49
2:D:24:ARG:HG3	2:D:24:ARG:NH1	2.26	0.49
2:N:195:ALA:O	2:N:199:GLN:CG	2.59	0.49
2:B:117:VAL:HG12	2:B:227:PRO:HB2	1.94	0.49
2:H:154:LEU:HD23	2:H:154:LEU:C	2.32	0.49
3:K:80:THR:CG2	4:L:9:ILE:HG22	2.42	0.49
1:M:150:SER:HB3	1:M:157:ILE:HD12	1.94	0.49
1:A:18:LEU:HD11	1:A:20:LEU:HG	1.95	0.49
2:H:30:ASN:HB3	2:H:50:TYR:O	2.12	0.49
1:M:97:THR:O	1:M:97:THR:OG1	2.30	0.49
1:A:101:LEU:HD13	2:B:98:GLY:HA2	1.94	0.49
1:A:196:PRO:O	1:A:199:THR:CG2	2.61	0.49
1:C:18:LEU:HD11	1:C:20:LEU:HG	1.93	0.49
1:G:2:SER:H	1:G:25:SER:CB	2.26	0.49
1:M:136:CYS:HG	1:M:186:CYS:CB	2.26	0.49
1:A:32:LEU:HD23	1:A:92:VAL:HG12	1.95	0.49
1:A:152:ASP:O	1:A:152:ASP:OD1	2.30	0.49
1:C:3:VAL:HG13	1:C:22:CYS:SG	2.53	0.49
1:C:151:LYS:CG	1:C:152:ASP:N	2.75	0.49
2:N:86:THR:O	2:N:87:SER:CB	2.60	0.49
2:B:134:HIS:HD2	2:B:134:HIS:O	1.96	0.49
1:C:1:GLN:HA	1:C:25:SER:HB3	1.95	0.48
3:K:123:TYR:CD1	3:K:124:ILE:HG22	2.45	0.48
1:A:151:LYS:HD2	1:A:192:ASN:OD1	2.12	0.48
2:B:199:GLN:HA	2:B:239:ARG:O	2.13	0.48
3:I:147:TRP:NE1	4:J:8:ASP:O	2.37	0.48
2:H:127:PRO:HD2	2:H:198:TRP:CZ2	2.48	0.48
2:H:134:HIS:O	2:H:134:HIS:CD2	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:201:PRO:HD2	2:N:202:ARG:H	1.77	0.48
1:A:155:VAL:HG22	1:A:179:SER:HB2	1.95	0.48
2:D:142:CYS:HB2	2:D:156:TRP:CZ2	2.48	0.48
2:N:83:PRO:HA	2:N:110:VAL:CG2	2.43	0.48
2:N:14:VAL:CG2	2:N:114:LEU:HD21	2.42	0.48
3:Q:80:THR:OG1	4:R:9:ILE:HG21	2.12	0.48
1:G:152:ASP:OD1	1:G:152:ASP:O	2.30	0.48
2:H:88:LEU:HD21	2:H:90:PHE:CE2	2.48	0.48
3:K:28:VAL:HG21	3:K:171:TYR:CE2	2.48	0.48
3:Q:78:LEU:O	3:Q:82:LEU:HD13	2.13	0.48
1:C:6:PRO:CG	1:C:21:ARG:HB2	2.42	0.48
3:Q:130:LEU:HD23	3:Q:157:ARG:HG2	1.96	0.48
1:A:194:ILE:HD11	2:N:224:ARG:CA	2.44	0.48
3:K:78:LEU:O	3:K:82:LEU:HD13	2.12	0.48
1:A:24:TYR:HH	1:A:66:PHE:HE1	1.61	0.48
2:B:83:PRO:HA	2:B:110:VAL:CG2	2.44	0.48
3:I:42:ASN:ND2	3:I:44:ARG:HD2	2.29	0.48
1:C:149:GLN:HG3	1:C:150:SER:H	1.79	0.48
1:C:194:ILE:O	1:C:194:ILE:CG2	2.61	0.48
3:E:159:TYR:CZ	3:E:164:CYS:HB2	2.49	0.48
1:M:10:VAL:HG12	1:M:109:LEU:HD12	1.95	0.48
1:A:196:PRO:HB2	1:A:199:THR:HG22	1.95	0.48
3:Q:130:LEU:N	3:Q:130:LEU:CD1	2.76	0.48
1:A:196:PRO:O	1:A:199:THR:HG23	2.14	0.48
3:E:111:ARG:CG	3:E:112:GLY:N	2.77	0.48
3:I:128:GLU:O	3:I:130:LEU:HD13	2.14	0.47
1:G:70:ASP:O	1:G:71:SER:HB2	2.14	0.47
1:M:59:VAL:HG22	1:M:60:ASN:N	2.29	0.47
2:D:80:LEU:HD13	2:H:75:PHE:CG	2.49	0.47
1:G:18:LEU:HD11	1:G:20:LEU:HG	1.96	0.47
2:H:142:CYS:HB2	2:H:156:TRP:CH2	2.49	0.47
1:A:28:ALA:HA	1:A:29:THR:HA	1.68	0.47
1:C:82:TRP:HA	1:C:111:VAL:CG1	2.44	0.47
1:C:155:VAL:HG22	1:C:179:SER:HB2	1.96	0.47
1:G:199:THR:O	1:G:199:THR:OG1	2.30	0.47
2:B:134:HIS:O	2:B:134:HIS:CD2	2.68	0.47
3:Q:56:GLY:O	3:Q:59:TYR:HB3	2.14	0.47
3:Q:96:GLN:HG2	3:Q:97:ARG:N	2.29	0.47
3:I:27:TYR:HA	3:I:31:LYS:O	2.15	0.47
1:M:70:ASP:O	1:M:71:SER:HB2	2.14	0.47
2:N:29:HIS:HB3	2:N:94:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PRO:HG2	1:A:205:GLU:HB2	1.97	0.47
2:B:78:LEU:N	2:B:78:LEU:CD1	2.76	0.47
3:E:159:TYR:CE2	3:E:164:CYS:HB2	2.49	0.47
2:N:117:VAL:HG11	2:N:214:LEU:CD1	2.45	0.47
1:A:82:TRP:HD1	1:A:111:VAL:O	1.98	0.47
1:C:123:TYR:CE1	2:D:131:GLU:HA	2.50	0.47
1:C:70:ASP:O	1:C:71:SER:HB2	2.14	0.47
2:N:142:CYS:HB2	2:N:156:TRP:CH2	2.50	0.47
1:A:142:ASP:OD1	1:A:145:THR:OG1	2.28	0.47
1:C:1:GLN:OE1	1:C:27:SER:HB2	2.14	0.47
2:D:117:VAL:HG11	2:D:214:LEU:CD1	2.45	0.47
3:E:56:GLY:O	3:E:59:TYR:HB3	2.14	0.47
1:G:32:LEU:HD23	1:G:92:VAL:HG12	1.97	0.47
2:N:240:ALA:O	2:N:241:ASP:C	2.53	0.47
1:G:194:ILE:O	1:G:194:ILE:CG2	2.61	0.46
1:M:32:LEU:HD23	1:M:92:VAL:HG12	1.97	0.46
1:A:122:VAL:HG12	1:A:122:VAL:O	2.13	0.46
1:C:59:VAL:HG22	1:C:60:ASN:N	2.30	0.46
2:D:30:ASN:HB3	2:D:50:TYR:O	2.15	0.46
2:D:127:PRO:HD2	2:D:198:TRP:CZ2	2.50	0.46
1:G:170:PHE:CE2	2:H:137:LYS:HE3	2.49	0.46
2:H:47:HIS:CE1	2:H:61:PRO:HB2	2.51	0.46
2:B:150:ASP:O	2:B:150:ASP:CG	2.53	0.46
2:H:15:THR:HG23	2:H:83:PRO:HD3	1.97	0.46
3:I:130:LEU:N	3:I:130:LEU:HD12	2.29	0.46
2:N:86:THR:O	2:N:87:SER:HB2	2.15	0.46
1:A:97:THR:HG22	1:A:97:THR:O	2.14	0.46
1:C:95:LYS:NZ	4:F:2:LEU:O	2.32	0.46
1:M:170:PHE:CE2	2:N:137:LYS:HE3	2.50	0.46
2:D:62:ASP:HB3	2:H:70:THR:HG22	1.96	0.46
3:E:14:ARG:CD	3:E:19:GLU:O	2.64	0.46
3:Q:133:TRP:HB2	3:Q:144:ARG:HG3	1.98	0.46
1:C:26:TYR:CD2	1:C:26:TYR:C	2.88	0.46
3:K:13:SER:HB3	3:K:78:LEU:HD13	1.97	0.46
1:C:137:LEU:HD12	1:C:175:ALA:O	2.16	0.46
3:E:19:GLU:HG3	3:E:75:ARG:NH1	2.30	0.46
3:K:167:TRP:CE2	4:L:1:PHE:HB3	2.51	0.46
1:M:29:THR:O	1:M:29:THR:OG1	2.30	0.46
1:A:62:PHE:CD2	1:A:75:LEU:HD11	2.50	0.46
2:D:83:PRO:CA	2:D:110:VAL:CG2	2.92	0.46
1:G:46:LEU:HD12	1:G:46:LEU:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:138:MET:O	3:Q:141:GLN:HB2	2.15	0.46
1:C:10:VAL:HG12	1:C:109:LEU:HD12	1.98	0.46
1:C:127:ASP:HB3	1:C:130:SER:O	2.16	0.46
2:D:82:SER:O	2:D:110:VAL:HG21	2.15	0.46
3:E:147:TRP:HB3	3:E:152:ALA:HB3	1.98	0.46
1:G:2:SER:H	1:G:25:SER:HB3	1.81	0.46
2:H:31:TYR:HA	2:H:49:SER:O	2.16	0.46
1:M:128:SER:HB2	2:N:126:GLU:OE2	2.16	0.46
2:B:169:THR:O	2:B:170:ASP:C	2.54	0.45
3:I:15:ARG:H	3:I:15:ARG:CZ	2.30	0.45
2:D:71:GLN:O	2:D:71:GLN:HG3	2.13	0.45
1:G:82:TRP:HA	1:G:111:VAL:CG1	2.46	0.45
2:H:124:VAL:HG23	2:H:234:ALA:HB3	1.97	0.45
1:M:47:LEU:HB2	1:M:56:VAL:HG11	1.98	0.45
2:N:47:HIS:CE1	2:N:61:PRO:HB2	2.51	0.45
3:Q:14:ARG:CD	3:Q:19:GLU:O	2.65	0.45
1:A:116:GLN:H	1:A:116:GLN:CD	2.20	0.45
2:B:177:GLN:O	2:B:183:SER:HB2	2.17	0.45
1:G:10:VAL:HG12	1:G:109:LEU:HD12	1.98	0.45
2:H:167:VAL:HG22	2:H:191:LEU:HD13	1.99	0.45
3:I:45:TYR:CE2	3:I:63:ILE:HG22	2.51	0.45
3:I:78:LEU:O	3:I:82:LEU:HD13	2.16	0.45
1:C:51:SER:HB3	3:E:158:ALA:HB2	1.97	0.45
2:D:220:TRP:HB2	2:D:226:LYS:HG3	1.99	0.45
2:B:114:LEU:HD13	2:B:214:LEU:HD21	1.98	0.45
2:D:114:LEU:HD22	2:D:214:LEU:HD21	1.98	0.45
3:K:174:ASN:OD1	3:K:174:ASN:N	2.50	0.45
2:B:24:ARG:HG3	2:B:24:ARG:NH1	2.32	0.45
1:A:120:PRO:CB	1:A:199:THR:HB	2.45	0.45
2:B:220:TRP:CB	2:B:226:LYS:HG3	2.47	0.45
1:G:116:GLN:CD	1:G:116:GLN:H	2.20	0.45
2:H:201:PRO:HB3	2:H:238:GLY:O	2.16	0.45
3:Q:8:TYR:CE1	3:Q:98:MET:HG3	2.52	0.45
3:Q:23:THR:HG23	3:Q:24:SER:N	2.31	0.45
1:A:120:PRO:HB2	1:A:199:THR:CA	2.47	0.45
3:E:15:ARG:HD3	3:Q:61:GLU:HG2	1.99	0.45
3:I:54:GLN:O	3:I:55:GLU:HG2	2.16	0.45
3:E:175:GLY:O	3:E:176:ASN:ND2	2.50	0.45
1:A:10:VAL:HG12	1:A:109:LEU:HD12	1.98	0.45
2:N:24:ARG:HG3	2:N:24:ARG:HH11	1.82	0.45
3:I:49:VAL:HG12	3:I:52:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:156:TYR:OH	4:J:5:PHE:HA	2.18	0.44
1:C:96:GLY:HA2	3:E:66:VAL:HG13	1.98	0.44
2:D:169:THR:HG23	2:D:189:SER:HB2	1.99	0.44
1:M:198:ASP:OD2	1:M:198:ASP:O	2.35	0.44
2:N:158:VAL:HB	2:N:163:VAL:HG11	1.98	0.44
1:A:105:LYS:HG3	1:A:106:GLY:N	2.32	0.44
1:M:133:LYS:HD2	1:M:133:LYS:HA	1.67	0.44
2:H:220:TRP:CB	2:H:226:LYS:HG3	2.48	0.44
1:C:122:VAL:HG12	1:C:122:VAL:O	2.16	0.44
2:D:167:VAL:CG2	2:D:191:LEU:HD13	2.48	0.44
2:H:87:SER:OG	2:H:88:LEU:N	2.50	0.44
2:H:132:ILE:HG23	2:H:195:ALA:CB	2.47	0.44
1:M:46:LEU:HD12	1:M:46:LEU:HA	1.72	0.44
1:M:49:TYR:CE2	1:M:66:PHE:CD2	3.05	0.44
1:M:152:ASP:OD2	1:M:154:ASP:HB2	2.18	0.44
2:N:10:ASN:OD1	2:N:151:HIS:NE2	2.39	0.44
2:N:220:TRP:HB2	2:N:226:LYS:HG3	1.99	0.44
3:Q:73:TRP:CE2	3:Q:77:ASN:ND2	2.85	0.44
1:A:137:LEU:HD12	1:A:175:ALA:O	2.18	0.44
3:I:77:ASN:OD1	4:J:9:ILE:HG12	2.18	0.44
1:C:156:TYR:O	1:C:177:ALA:HA	2.18	0.44
3:E:78:LEU:O	3:E:82:LEU:HD13	2.18	0.44
1:G:11:THR:HG23	1:G:110:THR:HB	1.99	0.44
1:M:116:GLN:H	1:M:116:GLN:CD	2.21	0.44
1:A:120:PRO:HB2	1:A:199:THR:CB	2.47	0.44
1:A:128:SER:HB3	2:B:126:GLU:HG3	2.00	0.44
2:B:50:TYR:CE2	2:B:56:GLN:HG3	2.50	0.44
1:G:156:TYR:O	1:G:177:ALA:HA	2.18	0.44
3:I:49:VAL:HG12	3:I:52:MET:CG	2.48	0.44
1:C:1:GLN:OE1	1:C:27:SER:CB	2.66	0.44
1:G:62:PHE:CD2	1:G:75:LEU:HD11	2.52	0.44
1:M:137:LEU:O	1:M:137:LEU:HG	2.18	0.44
3:Q:40:ALA:O	3:Q:41:GLU:C	2.53	0.44
2:B:9:ARG:NH2	2:B:153:GLU:OE2	2.35	0.44
1:C:149:GLN:CG	1:C:150:SER:N	2.80	0.44
3:K:47:PRO:HB3	3:K:52:MET:HB3	1.98	0.44
1:M:123:TYR:HB3	2:N:128:SER:CB	2.48	0.44
2:B:154:LEU:HD23	2:B:155:SER:N	2.33	0.44
1:C:49:TYR:CE2	1:C:66:PHE:CD2	3.06	0.44
2:H:156:TRP:CD1	2:H:167:VAL:HG13	2.52	0.44
3:I:19:GLU:CG	3:I:20:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:ASP:OD1	1:G:119:ASP:C	2.56	0.43
2:H:240:ALA:O	2:H:241:ASP:C	2.56	0.43
3:Q:156:TYR:HH	4:R:5:PHE:HA	1.83	0.43
3:I:56:GLY:O	3:I:59:TYR:HB3	2.18	0.43
3:I:147:TRP:CZ2	4:J:5:PHE:CZ	3.06	0.43
2:H:220:TRP:HB2	2:H:226:LYS:HG3	2.00	0.43
1:M:95:LYS:NZ	4:R:2:LEU:O	2.51	0.43
3:I:147:TRP:CZ2	4:J:5:PHE:HZ	2.35	0.43
1:C:0:ALA:O	1:C:1:GLN:C	2.53	0.43
1:G:32:LEU:HD13	1:G:73:PHE:HB2	2.01	0.43
3:Q:129:ASP:O	3:Q:130:LEU:HB2	2.17	0.43
2:B:47:HIS:CE1	2:B:61:PRO:HB2	2.52	0.43
2:D:240:ALA:O	2:D:241:ASP:C	2.56	0.43
3:K:54:GLN:O	3:K:54:GLN:CG	2.59	0.43
3:Q:80:THR:OG1	4:R:9:ILE:CG2	2.66	0.43
3:I:49:VAL:HA	3:I:50:PRO:HD3	1.93	0.43
1:C:33:PHE:CZ	2:D:98:GLY:HA3	2.53	0.43
1:G:192:ASN:O	1:G:192:ASN:ND2	2.51	0.43
3:K:15:ARG:H	3:K:15:ARG:HG3	1.51	0.43
1:M:16:ALA:O	1:M:80:VAL:HG22	2.17	0.43
1:C:62:PHE:CD2	1:C:75:LEU:HD11	2.53	0.43
3:I:8:TYR:O	3:I:24:SER:HA	2.19	0.43
1:C:95:LYS:HZ2	4:F:3:SER:HA	1.83	0.43
1:M:33:PHE:CZ	2:N:98:GLY:HA3	2.54	0.43
2:N:168:CYS:HB3	2:N:190:ARG:HD2	2.01	0.43
3:Q:61:GLU:O	3:Q:62:ARG:C	2.57	0.43
1:C:97:THR:O	1:C:97:THR:OG1	2.36	0.43
2:N:201:PRO:CD	2:N:202:ARG:N	2.82	0.43
1:A:197:GLU:HB3	2:D:228:VAL:HG21	2.00	0.43
2:D:114:LEU:HD13	2:D:214:LEU:HD21	2.00	0.43
1:M:6:PRO:CG	1:M:21:ARG:HB2	2.44	0.43
2:N:132:ILE:HG23	2:N:195:ALA:CB	2.48	0.43
3:K:17:LEU:CD1	3:K:75:ARG:HH21	2.31	0.42
4:R:9:ILE:HD12	4:R:9:ILE:HA	1.65	0.42
2:B:127:PRO:HD2	2:B:198:TRP:CZ2	2.54	0.42
3:E:23:THR:O	3:E:23:THR:HG22	2.19	0.42
1:G:31:TYR:CE2	3:K:155:TYR:CE1	3.08	0.42
3:K:23:THR:O	3:K:23:THR:HG22	2.18	0.42
1:A:6:PRO:CG	1:A:21:ARG:HB2	2.46	0.42
2:B:86:THR:O	2:B:87:SER:HB2	2.20	0.42
1:C:46:LEU:HD12	1:C:46:LEU:HA	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:127:ASN:O	3:I:130:LEU:HD12	2.19	0.42
1:A:203:SER:HB2	1:A:204:PRO:CD	2.50	0.42
3:I:96:GLN:HG2	3:I:97:ARG:N	2.34	0.42
1:C:116:GLN:CD	1:C:116:GLN:H	2.22	0.42
1:C:163:LEU:HB3	2:D:168:CYS:HB2	2.01	0.42
2:D:169:THR:O	2:D:170:ASP:C	2.55	0.42
3:K:49:VAL:HG12	3:K:52:MET:HG2	2.02	0.42
3:Q:5:MET:CE	3:Q:167:TRP:CE3	3.02	0.42
1:A:70:ASP:CB	1:A:72:SER:HB2	2.48	0.42
1:A:152:ASP:O	1:A:153:SER:OG	2.30	0.42
2:B:150:ASP:OD2	2:B:173:PRO:HG3	2.19	0.42
2:D:158:VAL:HB	2:D:163:VAL:HG11	2.01	0.42
1:G:34:TRP:CE2	1:G:75:LEU:HB2	2.55	0.42
2:H:175:LYS:HD3	2:H:183:SER:HB3	2.02	0.42
3:K:16:GLY:HA3	3:K:18:GLY:N	2.35	0.42
2:B:31:TYR:HA	2:B:49:SER:O	2.19	0.42
3:I:129:ASP:O	3:I:130:LEU:HB2	2.19	0.42
1:C:29:THR:CG2	3:E:163:GLU:HB2	2.49	0.42
2:H:114:LEU:HD22	2:H:214:LEU:HD21	2.02	0.42
2:N:51:GLY:HA3	3:Q:76:VAL:HG21	2.02	0.42
2:N:78:LEU:N	2:N:78:LEU:CD1	2.82	0.42
3:K:169:HIS:O	3:K:170:ARG:C	2.57	0.42
1:M:17:SER:HA	1:M:78:ALA:O	2.20	0.42
3:Q:19:GLU:CG	3:Q:20:PRO:HD2	2.34	0.42
1:A:138:PHE:HB2	1:A:190:PHE:CZ	2.55	0.42
3:I:23:THR:HG23	3:I:24:SER:N	2.33	0.42
1:C:24:TYR:OH	1:C:66:PHE:HE1	2.02	0.42
1:C:149:GLN:CG	1:C:150:SER:H	2.32	0.42
2:H:169:THR:HG23	2:H:189:SER:HB2	2.02	0.42
1:A:127:ASP:HB2	1:A:133:LYS:HB2	2.00	0.41
3:E:155:TYR:CD2	3:E:156:TYR:CE2	3.08	0.41
2:H:231:ILE:HG22	2:H:232:VAL:N	2.35	0.41
3:K:171:TYR:CD2	3:K:171:TYR:C	2.93	0.41
1:M:141:PHE:CZ	1:M:173:ASN:HB3	2.55	0.41
3:Q:13:SER:HB3	3:Q:78:LEU:HD13	2.01	0.41
1:G:6:PRO:CG	1:G:21:ARG:HB2	2.49	0.41
3:I:111:ARG:HG2	3:I:113:TYR:CZ	2.55	0.41
2:N:142:CYS:HB2	2:N:156:TRP:CZ2	2.55	0.41
2:B:57:ILE:CG1	2:B:61:PRO:HG3	2.51	0.41
2:D:15:THR:HG23	2:D:83:PRO:HD3	2.01	0.41
3:Q:147:TRP:HB3	3:Q:152:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:220:TRP:CB	2:D:226:LYS:HG3	2.50	0.41
2:H:169:THR:O	2:H:170:ASP:C	2.58	0.41
2:D:117:VAL:HG11	2:D:214:LEU:HD12	2.03	0.41
1:G:70:ASP:CB	1:G:72:SER:HB2	2.48	0.41
1:G:166:ARG:HE	1:G:166:ARG:HB2	1.61	0.41
2:N:181:ASN:OD1	2:N:181:ASN:N	2.53	0.41
1:A:133:LYS:HD2	1:A:133:LYS:HA	1.76	0.41
2:D:101:TYR:CD2	2:D:101:TYR:N	2.89	0.41
1:M:125:LEU:HB3	2:N:126:GLU:O	2.21	0.41
2:N:220:TRP:CB	2:N:226:LYS:HG3	2.51	0.41
3:Q:61:GLU:O	3:Q:64:THR:N	2.53	0.41
1:A:82:TRP:HA	1:A:111:VAL:CG1	2.50	0.41
1:A:113:PRO:O	1:A:143:SER:OG	2.39	0.41
2:B:220:TRP:HB2	2:B:226:LYS:HG3	2.02	0.41
3:I:147:TRP:HB3	3:I:152:ALA:HB3	2.03	0.41
1:C:133:LYS:HD2	1:C:133:LYS:HA	1.72	0.41
2:D:201:PRO:HB3	2:D:238:GLY:O	2.21	0.41
3:E:8:TYR:CE1	3:E:98:MET:HG3	2.56	0.41
1:G:136:CYS:SG	1:G:184:PHE:CE2	3.13	0.41
1:M:62:PHE:CD2	1:M:75:LEU:HD11	2.55	0.41
2:N:124:VAL:HG23	2:N:234:ALA:HB3	2.03	0.41
2:B:82:SER:O	2:B:110:VAL:HG21	2.20	0.41
1:C:183:ASP:OD1	1:C:183:ASP:O	2.38	0.41
2:D:154:LEU:HD23	2:D:155:SER:N	2.36	0.41
1:C:3:VAL:CG1	1:C:22:CYS:SG	3.09	0.40
1:G:59:VAL:HG22	1:G:60:ASN:H	1.86	0.40
2:H:220:TRP:CG	2:H:226:LYS:HG3	2.56	0.40
3:K:45:TYR:CE2	3:K:63:ILE:HG22	2.56	0.40
1:M:34:TRP:CE2	1:M:75:LEU:HB2	2.56	0.40
3:E:58:GLU:HA	3:E:61:GLU:HB2	2.03	0.40
2:B:142:CYS:HB2	2:B:156:TRP:CH2	2.57	0.40
3:I:130:LEU:HD23	3:I:157:ARG:HG2	2.02	0.40
1:C:115:ILE:O	1:C:118:PRO:HD3	2.22	0.40
3:E:23:THR:HG23	3:E:24:SER:N	2.36	0.40
2:H:86:THR:O	2:H:87:SER:HB2	2.22	0.40
1:C:38:TYR:CD1	1:C:86:ALA:HB2	2.56	0.40
1:C:119:ASP:O	1:C:140:ASP:HB2	2.21	0.40
2:D:126:GLU:HA	2:D:127:PRO:HD3	1.89	0.40
2:D:164:HIS:N	5:D:242:SO4:O2	2.52	0.40
1:G:38:TYR:CD1	1:G:86:ALA:HB2	2.57	0.40
3:K:78:LEU:HD23	3:K:78:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:127:ASP:HB2	1:M:133:LYS:HB2	2.03	0.40
3:Q:5:MET:SD	3:Q:167:TRP:CE3	3.15	0.40
4:R:2:LEU:HD23	4:R:2:LEU:HA	1.75	0.40
1:C:192:ASN:O	1:C:192:ASN:ND2	2.54	0.40
2:D:9:ARG:HH12	2:D:153:GLU:CD	2.22	0.40
3:E:45:TYR:CE2	3:E:63:ILE:HG22	2.56	0.40
1:G:97:THR:O	1:G:97:THR:OG1	2.35	0.40
3:K:133:TRP:HB2	3:K:144:ARG:HG3	2.03	0.40
3:Q:34:VAL:CG2	3:Q:35:ARG:N	2.85	0.40
3:Q:78:LEU:HD23	3:Q:78:LEU:HA	1.91	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:167:SER:O	2:N:136:GLN:NE2[2_555]	2.03	0.17

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	201/211 (95%)	183 (91%)	16 (8%)	2 (1%)	15 49
1	C	202/211 (96%)	184 (91%)	18 (9%)	0	100 100
1	G	198/211 (94%)	181 (91%)	15 (8%)	2 (1%)	15 49
1	M	202/211 (96%)	189 (94%)	13 (6%)	0	100 100
2	B	238/243 (98%)	223 (94%)	15 (6%)	0	100 100
2	D	238/243 (98%)	225 (94%)	13 (6%)	0	100 100
2	H	238/243 (98%)	224 (94%)	14 (6%)	0	100 100
2	N	238/243 (98%)	226 (95%)	11 (5%)	1 (0%)	34 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	171/180 (95%)	160 (94%)	11 (6%)	0	100	100
3	I	169/180 (94%)	158 (94%)	11 (6%)	0	100	100
3	K	173/180 (96%)	158 (91%)	15 (9%)	0	100	100
3	Q	174/180 (97%)	161 (92%)	12 (7%)	1 (1%)	25	59
4	F	7/9 (78%)	7 (100%)	0	0	100	100
4	J	7/9 (78%)	7 (100%)	0	0	100	100
4	L	7/9 (78%)	7 (100%)	0	0	100	100
4	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	2470/2572 (96%)	2299 (93%)	165 (7%)	6 (0%)	47	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	PHE
3	Q	43	PRO
2	N	87	SER
1	G	94	ALA
1	A	39	PRO
1	G	39	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/186 (97%)	169 (94%)	11 (6%)	18	49
1	C	178/186 (96%)	166 (93%)	12 (7%)	16	46
1	G	177/186 (95%)	167 (94%)	10 (6%)	21	52
1	M	179/186 (96%)	171 (96%)	8 (4%)	27	60
2	B	206/208 (99%)	199 (97%)	7 (3%)	37	69
2	D	206/208 (99%)	198 (96%)	8 (4%)	32	65
2	H	206/208 (99%)	200 (97%)	6 (3%)	42	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	N	206/208 (99%)	198 (96%)	8 (4%)	32 65
3	E	144/148 (97%)	140 (97%)	4 (3%)	43 73
3	I	143/148 (97%)	137 (96%)	6 (4%)	30 62
3	K	144/148 (97%)	136 (94%)	8 (6%)	21 52
3	Q	144/148 (97%)	140 (97%)	4 (3%)	43 73
4	F	9/9 (100%)	9 (100%)	0	100 100
4	J	9/9 (100%)	9 (100%)	0	100 100
4	L	9/9 (100%)	9 (100%)	0	100 100
4	R	9/9 (100%)	8 (89%)	1 (11%)	6 24
All	All	2149/2204 (98%)	2056 (96%)	93 (4%)	29 62

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	11	THR
1	A	26	TYR
1	A	65	GLU
1	A	99	SER
1	A	123	TYR
1	A	182	SER
1	A	183	ASP
1	A	199	THR
1	A	205	GLU
1	A	206	SER
2	B	9	ARG
2	B	38	ASP
2	B	71	GLN
2	B	110	VAL
2	B	112	GLU
2	B	190	ARG
2	B	241	ASP
3	I	15	ARG
3	I	23	THR
3	I	28	VAL
3	I	49	VAL
3	I	86	ASN
3	I	111	ARG
1	C	4	THR

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Mol	Chain	Res	Type
1	C	26	TYR
1	C	29	THR
1	C	65	GLU
1	C	81	HIS
1	C	95	LYS
1	C	97	THR
1	C	135	VAL
1	C	138	PHE
1	C	151	LYS
1	C	153	SER
1	C	186	CYS
2	D	9	ARG
2	D	71	GLN
2	D	110	VAL
2	D	112	GLU
2	D	190	ARG
2	D	210	GLN
2	D	239	ARG
2	D	241	ASP
3	E	23	THR
3	E	28	VAL
3	E	49	VAL
3	E	86	ASN
1	G	4	THR
1	G	11	THR
1	G	65	GLU
1	G	97	THR
1	G	123	TYR
1	G	134	SER
1	G	143	SER
1	G	197	GLU
1	G	199	THR
1	G	203	SER
2	H	71	GLN
2	H	110	VAL
2	H	112	GLU
2	H	187	LEU
2	H	190	ARG
2	H	241	ASP
3	K	5	MET
3	K	15	ARG
3	K	23	THR

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Mol	Chain	Res	Type
3	K	49	VAL
3	K	52	MET
3	K	86	ASN
3	K	111	ARG
3	K	174	ASN
1	M	4	THR
1	M	65	GLU
1	M	95	LYS
1	M	97	THR
1	M	131	SER
1	M	146	ASN
1	M	149	GLN
1	M	198	ASP
2	N	38	ASP
2	N	71	GLN
2	N	110	VAL
2	N	112	GLU
2	N	176	GLU
2	N	190	ARG
2	N	228	VAL
2	N	241	ASP
3	Q	15	ARG
3	Q	23	THR
3	Q	49	VAL
3	Q	86	ASN
4	R	9	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	47	HIS
2	B	134	HIS
2	B	177	GLN
3	I	127	ASN
3	E	176	ASN
2	H	47	HIS
2	H	134	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	K	180	-	4,4,4	0.18	0	6,6,6	0.39	0
5	SO4	K	181	-	4,4,4	0.98	0	6,6,6	1.66	1 (16%)
5	SO4	N	243	-	4,4,4	0.16	0	6,6,6	0.62	0
6	EDO	N	244	-	3,3,3	0.41	0	2,2,2	0.38	0
5	SO4	B	242	-	4,4,4	0.20	0	6,6,6	0.46	0
5	SO4	H	242	-	4,4,4	0.13	0	6,6,6	0.34	0
5	SO4	A	208	-	4,4,4	0.13	0	6,6,6	0.69	0
5	SO4	H	243	-	4,4,4	0.30	0	6,6,6	0.54	0
5	SO4	D	243	-	4,4,4	0.19	0	6,6,6	0.38	0
5	SO4	B	244	-	4,4,4	0.29	0	6,6,6	0.37	0
5	SO4	B	243	-	4,4,4	0.31	0	6,6,6	0.48	0
5	SO4	D	242	-	4,4,4	0.08	0	6,6,6	0.50	0
5	SO4	N	242	-	4,4,4	0.17	0	6,6,6	0.05	0
5	SO4	G	208	-	4,4,4	0.32	0	6,6,6	0.21	0
5	SO4	Q	180	-	4,4,4	0.23	0	6,6,6	0.33	0
5	SO4	E	180	-	4,4,4	0.26	0	6,6,6	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	N	244	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	181	SO4	O4-S-O3	3.83	125.39	109.06

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	244	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	243	SO4	3	0
5	H	243	SO4	1	0
5	D	242	SO4	1	0
5	E	180	SO4	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	205/211 (97%)	-0.02	0 100 100	42, 77, 113, 124	0
1	C	204/211 (96%)	0.21	2 (0%) 82 67	24, 81, 114, 125	0
1	G	202/211 (95%)	0.34	6 (2%) 50 27	44, 80, 119, 130	0
1	M	204/211 (96%)	0.37	4 (1%) 65 44	49, 82, 119, 140	0
2	B	240/243 (98%)	-0.34	1 (0%) 92 84	34, 54, 94, 130	0
2	D	240/243 (98%)	-0.40	0 100 100	32, 55, 95, 133	0
2	H	240/243 (98%)	-0.18	5 (2%) 63 43	33, 56, 100, 131	0
2	N	240/243 (98%)	-0.18	3 (1%) 77 59	34, 55, 100, 133	0
3	E	175/180 (97%)	-0.23	0 100 100	44, 61, 109, 155	0
3	I	173/180 (96%)	-0.22	1 (0%) 89 78	46, 64, 111, 154	0
3	K	175/180 (97%)	-0.18	0 100 100	43, 59, 113, 153	0
3	Q	176/180 (97%)	-0.17	3 (1%) 70 49	46, 64, 119, 137	0
4	F	9/9 (100%)	-0.29	0 100 100	45, 50, 55, 58	0
4	J	9/9 (100%)	-0.27	0 100 100	49, 54, 70, 71	0
4	L	9/9 (100%)	-0.16	0 100 100	39, 44, 52, 53	0
4	R	9/9 (100%)	-0.30	0 100 100	49, 55, 62, 65	0
All	All	2510/2572 (97%)	-0.09	25 (0%) 82 67	24, 66, 111, 155	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	202	PRO	3.5
3	Q	17	LEU	3.5
1	G	191	ASN	3.4
2	H	240	ALA	3.2
2	N	203	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	180	LEU	2.6
2	H	2	ALA	2.6
2	H	129	GLU	2.6
1	G	151	LYS	2.5
1	C	194	ILE	2.5
1	G	190	PHE	2.4
3	Q	41	GLU	2.4
1	M	132	ASP	2.4
1	M	150	SER	2.4
3	I	54	GLN	2.3
2	H	132	ILE	2.2
1	C	152	ASP	2.2
3	Q	89	ALA	2.1
1	M	190	PHE	2.1
1	G	147	VAL	2.1
1	G	96	GLY	2.1
2	N	241	ASP	2.1
2	B	205	PHE	2.0
1	M	194	ILE	2.0
2	N	181	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	208	5/5	0.80	0.25	78,93,101,101	5
5	SO4	N	243	5/5	0.85	0.25	91,98,118,124	5
5	SO4	B	244	5/5	0.86	0.30	49,62,74,75	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	H	243	5/5	0.90	0.12	86,88,91,118	0
5	SO4	B	243	5/5	0.90	0.20	79,83,100,128	0
5	SO4	E	180	5/5	0.92	0.19	60,68,75,77	5
5	SO4	G	208	5/5	0.92	0.17	45,56,62,76	5
5	SO4	Q	180	5/5	0.93	0.17	79,86,105,119	5
5	SO4	D	242	5/5	0.94	0.11	63,72,93,94	0
5	SO4	K	181	5/5	0.94	0.22	88,91,95,97	5
6	EDO	N	244	4/4	0.94	0.27	60,62,75,79	0
5	SO4	H	242	5/5	0.95	0.10	77,89,102,117	0
5	SO4	K	180	5/5	0.95	0.10	59,68,72,82	5
5	SO4	N	242	5/5	0.96	0.14	96,97,97,98	5
5	SO4	B	242	5/5	0.96	0.10	57,71,84,89	0
5	SO4	D	243	5/5	0.97	0.14	45,68,82,97	5

6.5 Other polymers

There are no such residues in this entry.